Quantum Loop Topography for Machine Learning Transport

Yi Zhang (Frank)
Cornell University

Motivated and enlightened @ KITP two years ago…

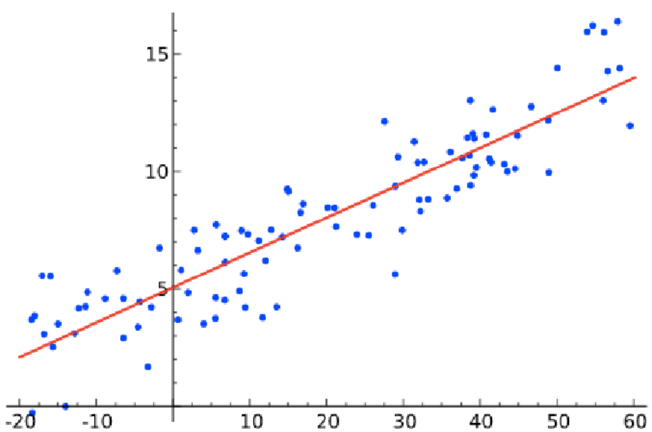
Selected for a Viewpoint in *Physics*
PRL **118,** 216401 (2017) PHYSICAL REVIEW LETTERS week ending 26 MAY 2017

Quantum Loop Topography for Machine Learning

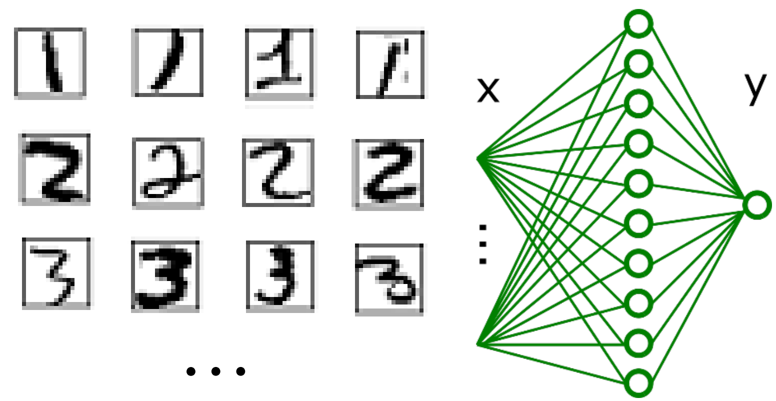
Yi Zhang[*] and Eun-Ah Kim[†]
Department of Physics, Cornell University, Ithaca, New York 14853, USA
and Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA

Machine learning (with artificial neural network)

Learn a function from data
(linear regression = least squares fit)



Learning a digit-recognition neural network from data
= the least cross-entropy cost (most answers correct)

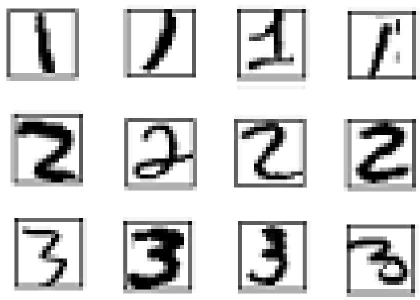


(1) Powerful, non-linear representation

(2) Efficient regression algorithm

Machine learning Condensed Matter Phases of Matter

Image



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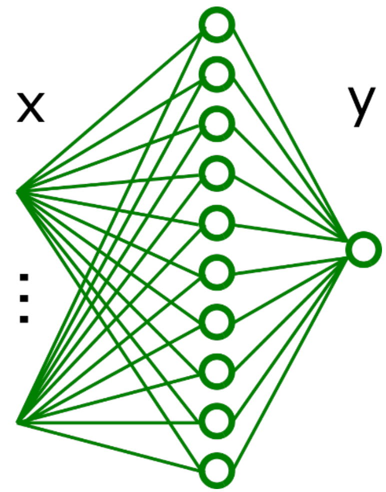


Category

1

2

3

Many-body state

Phase

Liquid

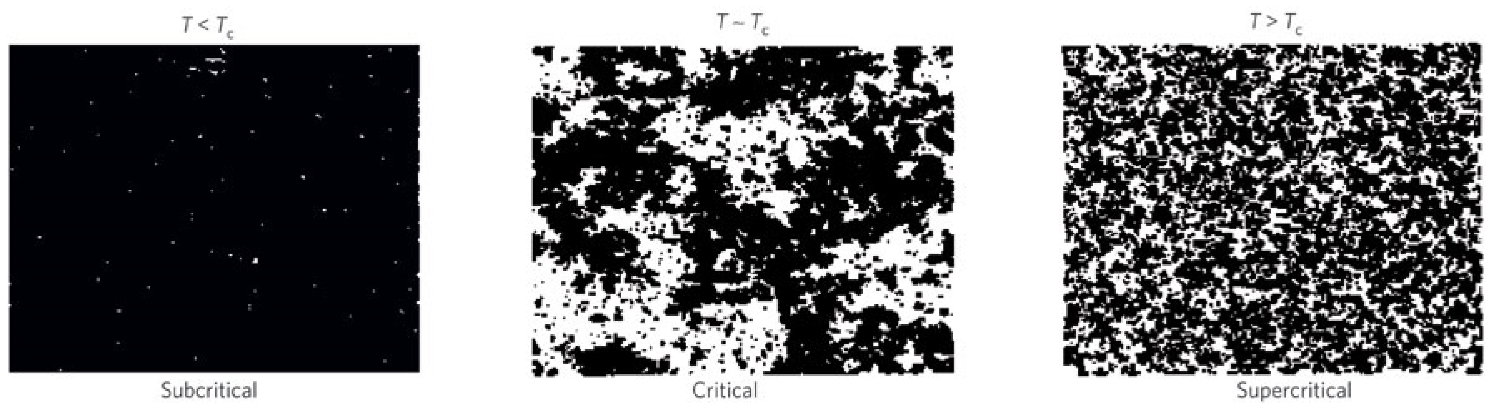
or

Solid

Machine learning Condensed Matter
Phases of Matter

- Machine learning phases of matter and phase transitions

What do we use as data?



Snapshots of the order parameter field for the 2D Ising model

J. Carrasquilla and R.G. Melko (2016)

Machine learning for quantum systems?

Generic quantum systems ⟷ ? ⟷ Machine learning architecture

- Local order parameter or conservation

  J. Carrasquilla, R.G. Melko (2016); L. Wang (2016); etc.

- Entanglement

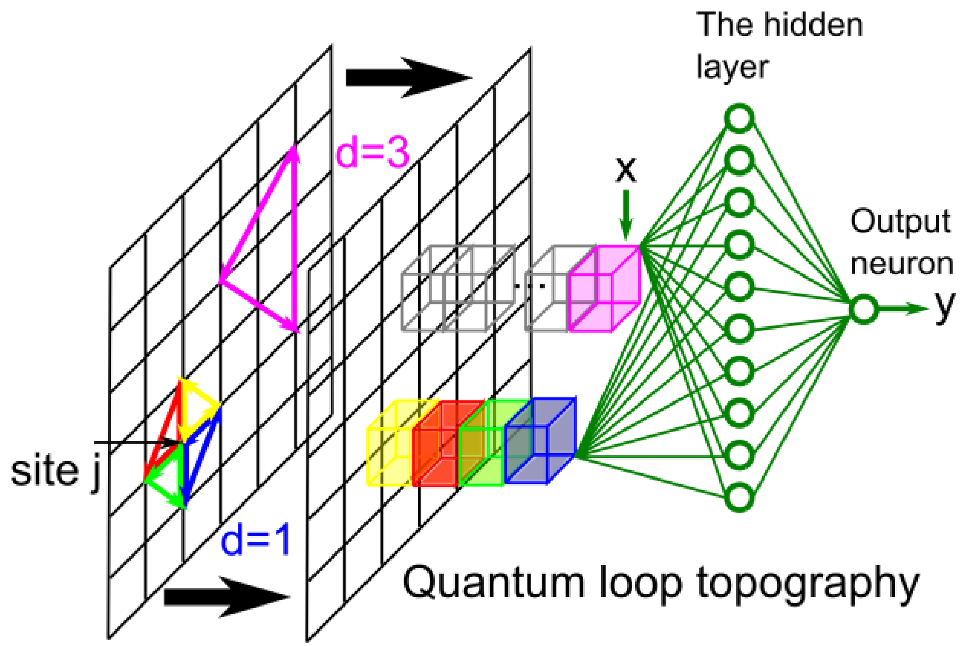
  E. P. L. van Nieuwenburg, Ye-Hua Liu, Sebastian D. Huber; Frank Schindler, Nicolas Regnault, Titus Neupert (2017); etc.*

- Correlation

  P. Broecker, J. Carrasquilla, R.G. Melko, S. Trebst (2017); etc.

MACHINE LEARNING WITH QUANTUM LOOP TOPOGRAPHY

Quantum operators for machine learning quantum systems



1. Physics inspired selections:

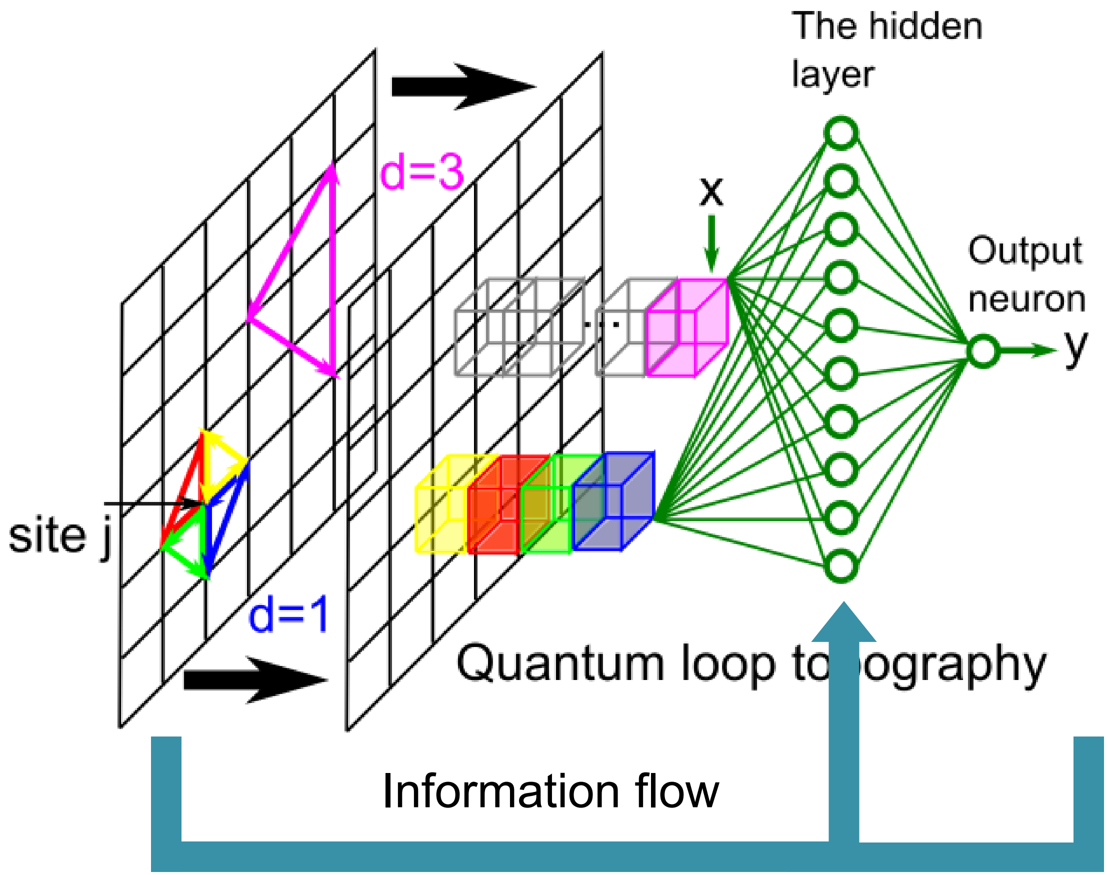
e.g. physical transport

Quantum system ⟷ 'Informative' operators ⟷ Machine learning algorithm

2. Interpretability – guiding principles

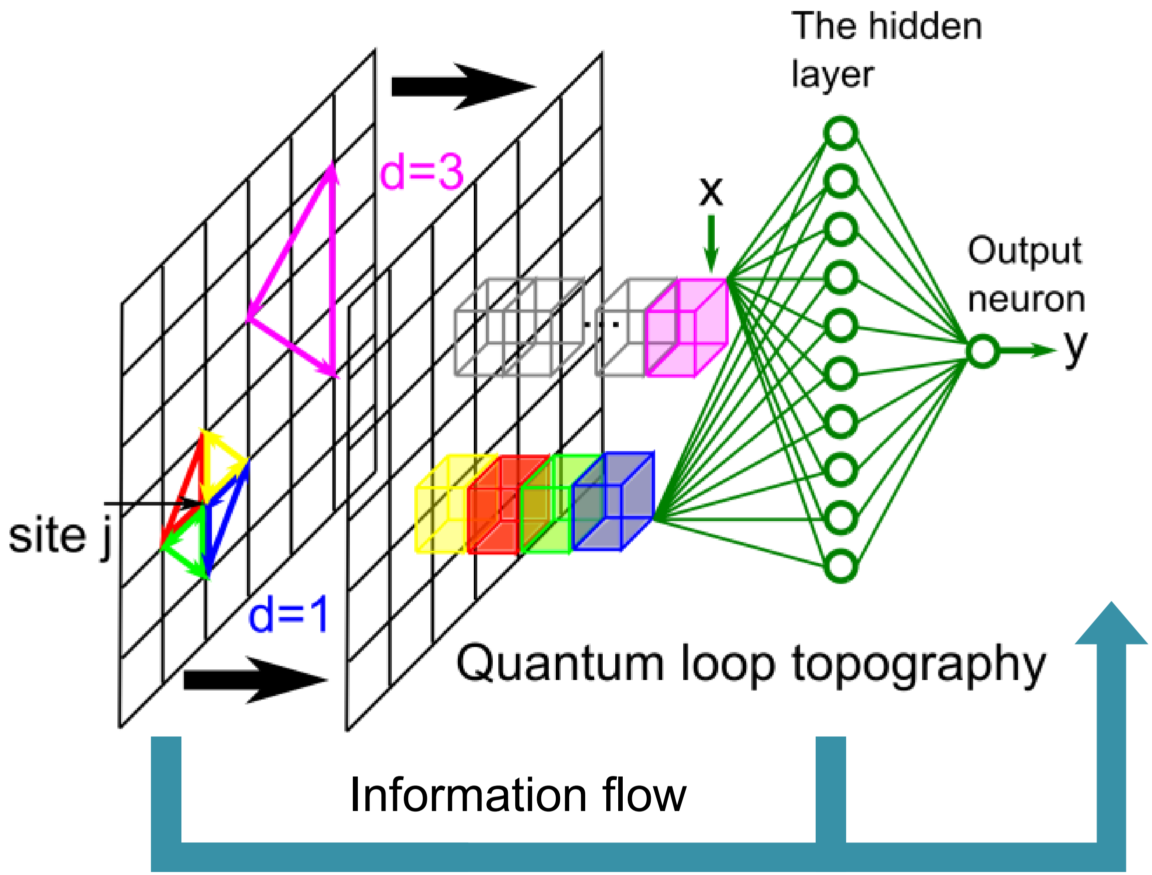
YZ, E.-A. Kim (2017)

Machine learning with quantum loop topography



- Training: using known, well-controlled examples to optimize the neural network

Machine learning with quantum loop topography



- Application: using the optimized neural network to identify the phases of the samples in question

Example #1: quantum Hall phases

Physics intuition on quantum Hall phases

- Q1. What is characteristic for the quantum Hall phases?
- A1. Hall transport!

- Q2. What are the related operators?
- A2. Kubo formula

$$\sigma_{xy} = \frac{ie^2\hbar}{N}\left[\sum_{n\neq 0}\frac{\langle\Phi_0|v_y|\Phi_n\rangle\langle\Phi_n|v_x|\Phi_0\rangle - x\leftrightarrow y}{(E_n-E_0)^2}\right]$$

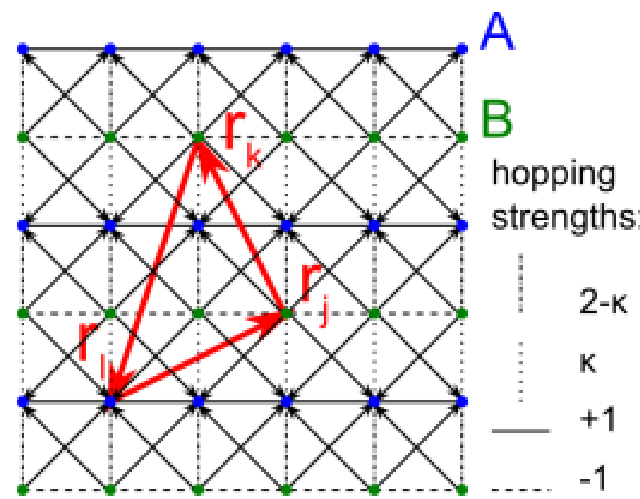
$$H' = -\Delta P \qquad P = \sum_{m\in v}|m\rangle\langle m| \qquad P_{ij}\equiv\langle c_i^\dagger c_j\rangle$$

$$\sigma_{xy} = \frac{e^2}{h}\cdot\frac{1}{N}\sum 4\pi i P_{jk}P_{kl}P_{lj}S_{\triangle jkl}$$

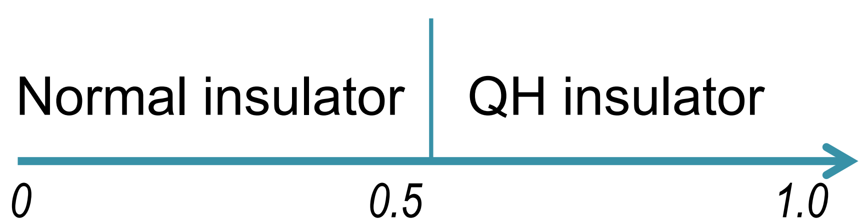
Raffaello Bianco and Raffaele Resta (2011).

Example: a non-interacting tight-binding model

$$H(\kappa) = \sum_{\vec{r}} (-1)^y c^\dagger_{\vec{r}+\hat{x}} c_{\vec{r}} + [1 + (-1)^y (1-\kappa)] c^\dagger_{\vec{r}+\hat{y}} c_{\vec{r}} + (-1)^y \frac{i\kappa}{2} [c^\dagger_{\vec{r}+\hat{x}+\hat{y}} c_{\vec{r}} + c^\dagger_{\vec{r}+\hat{x}-\hat{y}} c_{\vec{r}}] + \text{H.c.},$$



Gap changes sign
at phase transition

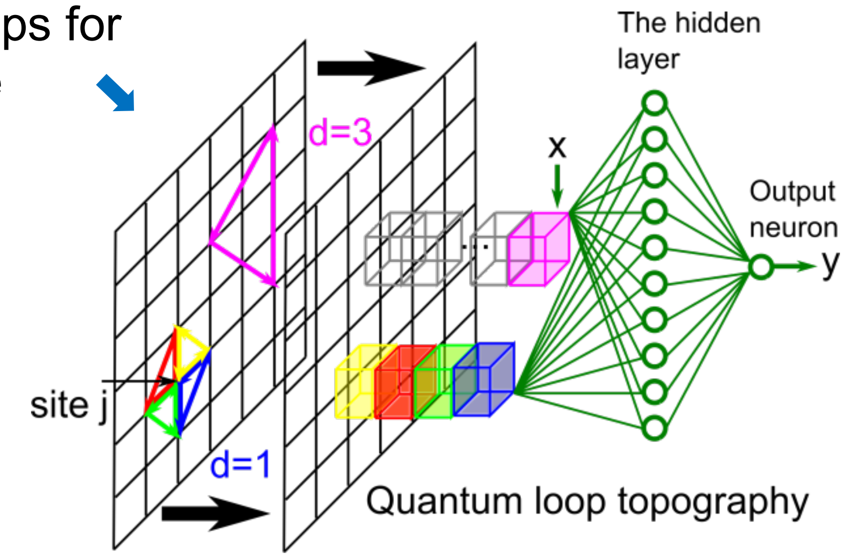


Tuning parameter κ:

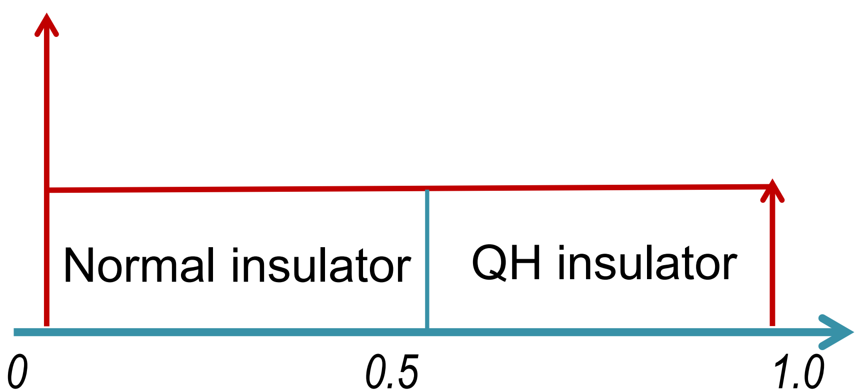
YZ, E.-A. Kim (2017)

Machine learning QH insulator

Triangular loops for Hall response

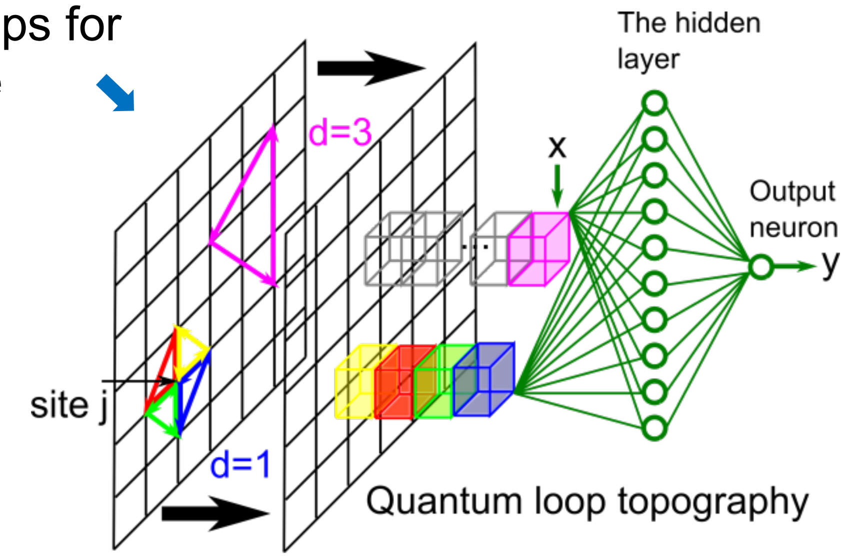


Tuning parameter κ:

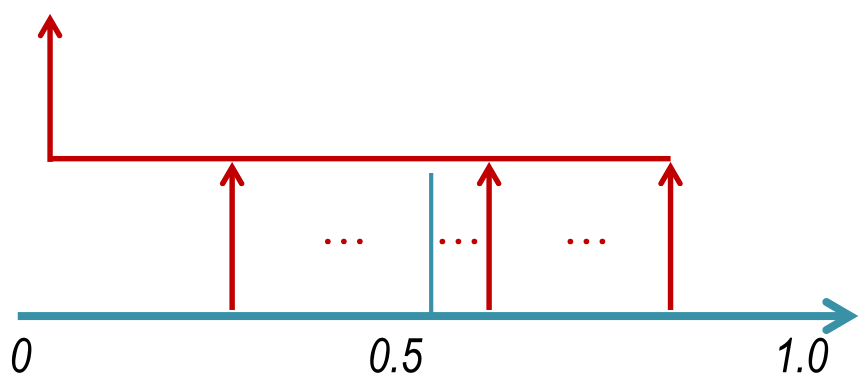


Machine learning QH insulator

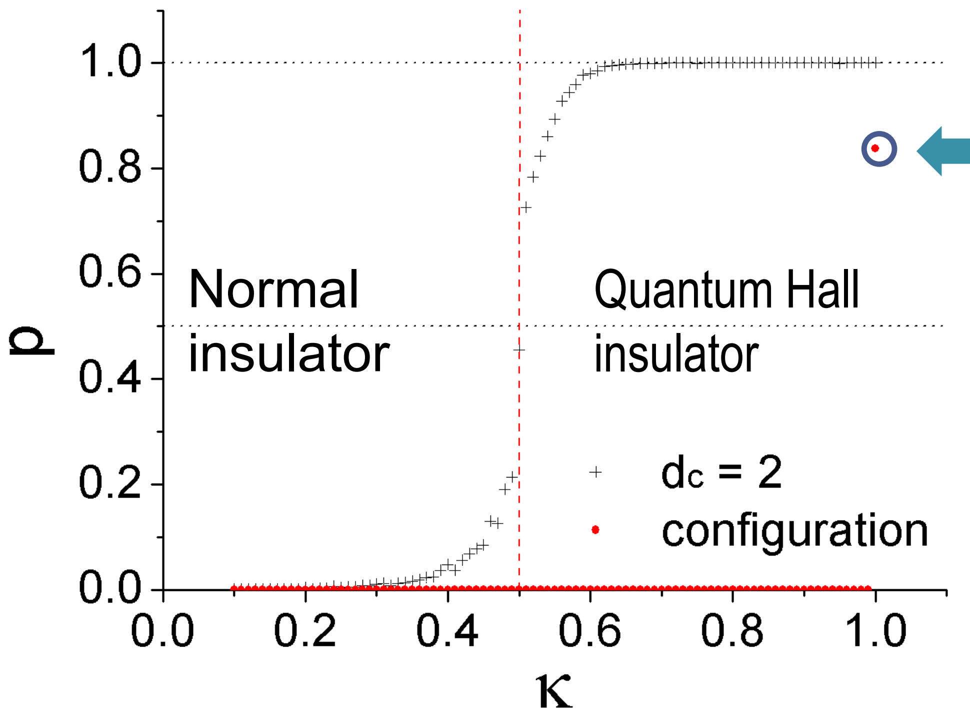
Triangular loops for Hall response



Tuning parameter κ:

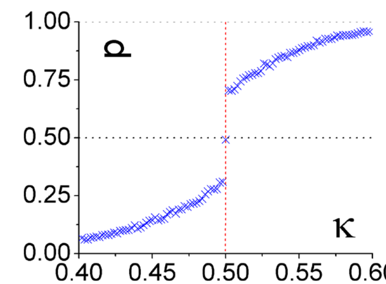


Phase diagram by machine learning

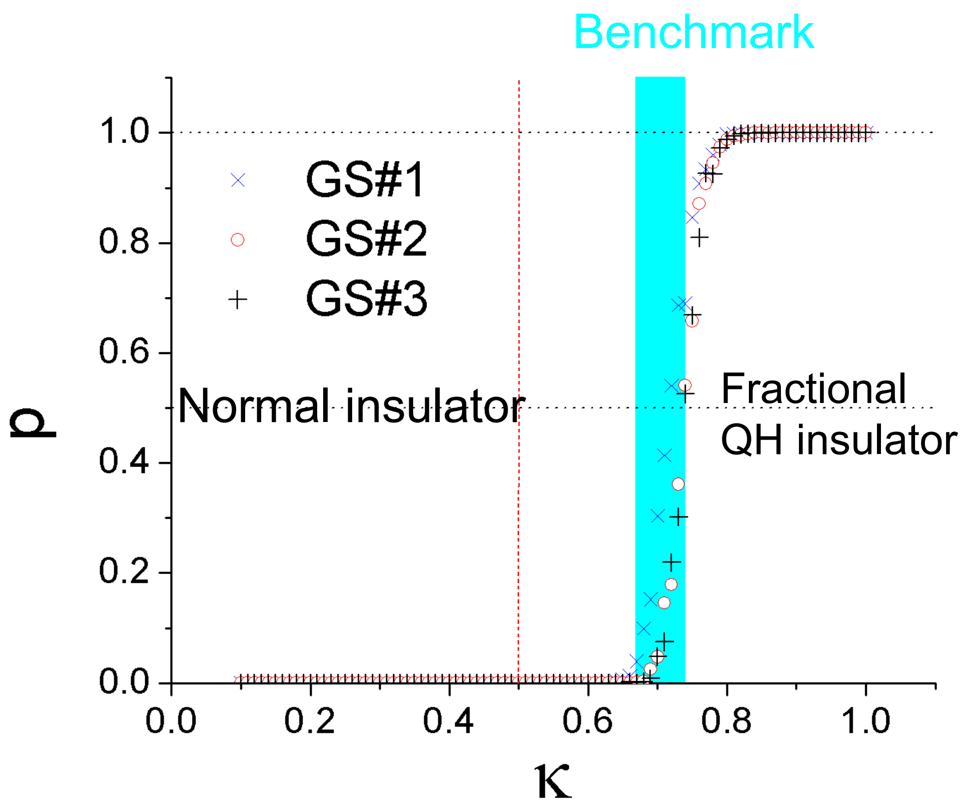


use the electron number operators

$$n_r = c_r^\dagger c_r$$



Also work for fractional QH phases



Also, correctly distinguish different topological phases (e.g. fractional vs integer QH insulators), and topological indices (e.g. ν=1 vs ν =-1).

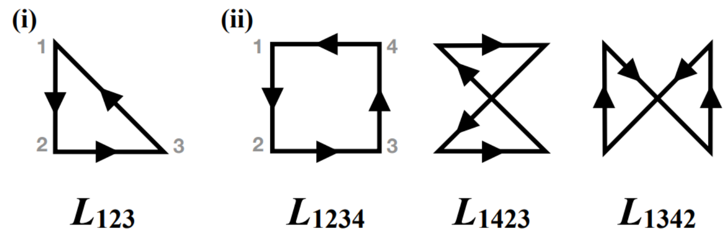
YZ, E.-A. Kim (2017)

Example #2: superconducting fluctuations

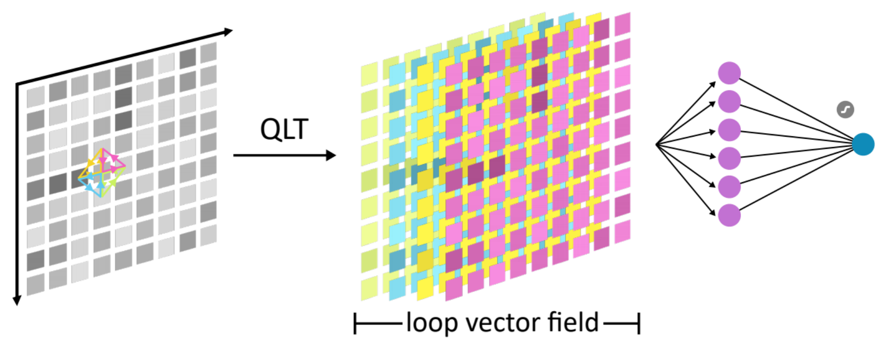
Physics intuition on longitudinal transport

- Dissemble current-current correlations:

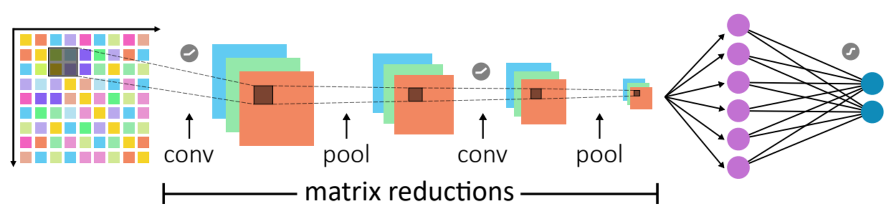
$$L_{ijkl} = [P_{ij}P_{jk}P_{kl}P_{li}]$$
$$L'_{jkl} = [P_{jk}P_{kl}P_{lj}]$$



- Let's compare QLT and CNN side by side:



Direct input of MC samples of two-point correlations P:



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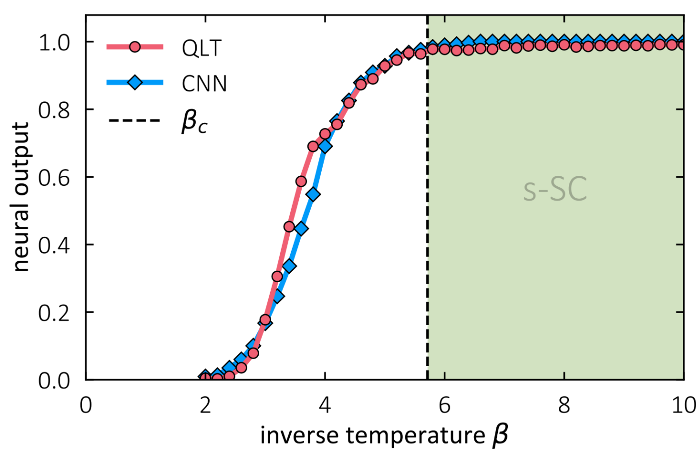
The negative-U Hubbard model phase diagram from machine learning

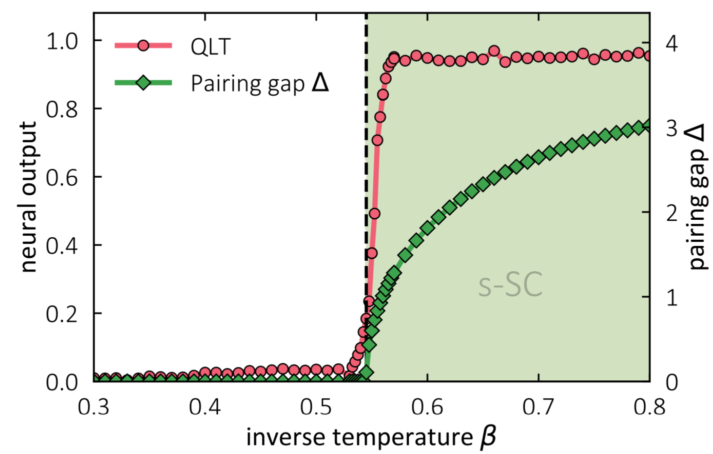
$$H = -\sum_{\langle ij \rangle, s} \left(c^\dagger_{j,s} c_{i,s} + c^\dagger_{i,s} c_{j,s} \right) - \mu \sum_i \left(n_{i,\uparrow} + n_{i,\downarrow} \right)$$
$$+ U \sum_i \left(n_{i,\uparrow} - \frac{1}{2} \right) \left(n_{i,\downarrow} - \frac{1}{2} \right)$$

- DQMC samples:



- KT-type transition
- sensitive to the onset of superconducting fluctuations

- Mean-field ansatz:



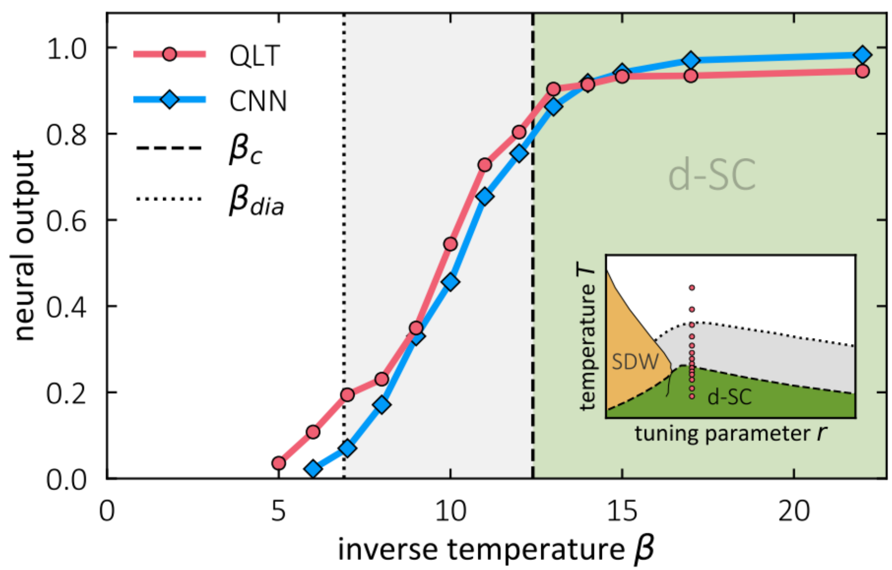
- No fluctuations
- Sharp signal when pairing gap opens

Also work for d-wave superconductivity

$$S_\psi = -\int_{\tau,\mathbf{r},\mathbf{r}'} \sum_{s,\alpha} \left[(\partial_\tau - \mu)\, \delta_{\mathbf{r}\mathbf{r}'} - t_{\alpha\mathbf{r}\mathbf{r}'} \right] \psi^\dagger_{\alpha\mathbf{r}s} \psi_{\alpha\mathbf{r}'s}$$

$$S_\lambda = \lambda \int_{\tau,\mathbf{r}} e^{i\mathbf{Q}\cdot\mathbf{r_i}} \vec{\varphi}_\mathbf{r} \cdot \left(\psi^\dagger_{a\mathbf{r}s} \vec{\sigma}_{ss'} \psi_{b\mathbf{r}s'} + \text{h.c.} \right)$$

$$S_\varphi = \int_{\tau,\mathbf{r}} \frac{1}{2c^2} \left(\partial_\tau \vec{\varphi}\right)^2 + \left(\nabla \vec{\varphi}\right)^2 + \frac{r}{2} \vec{\varphi}^2 + \frac{u}{4} (\vec{\varphi}^2)^2$$



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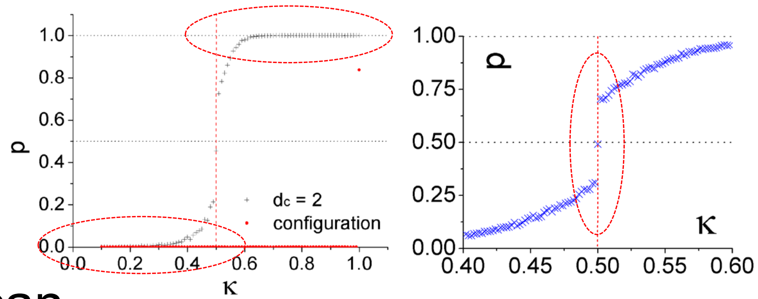
Advantages



- Accuracy
- Efficiency
  - automated phase-space scan
  - okay with Monte Carlo samples
  - okay with simpler machine learning scheme
- Versatility
  - lattice
  - symmetries and disorders
  - systematic ansatz
  - partial information

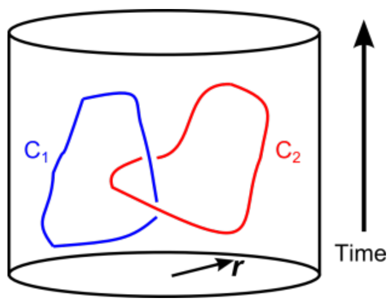
Disadvantages?

QUANTUM LOOP TOPOGRAPHY PHILOSOPHY

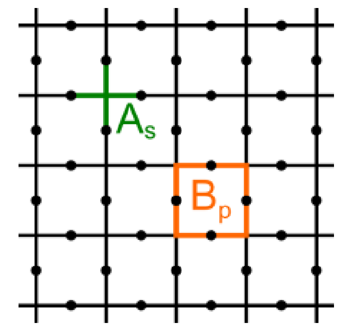
The 'good' versus the 'not-so-good'

- The 'good':

Topological quantum field theory:



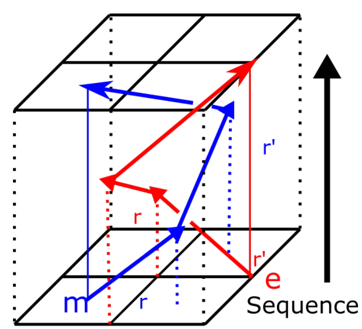
Exactly solvable lattice model:



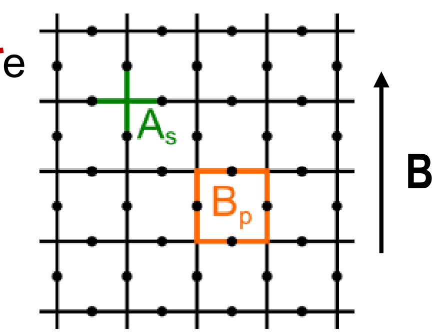
- The 'not-so-good':

Lattice model reality:

- Discrete lattice
- Finite correlation
- Cut off, fluctuation and uncertainty

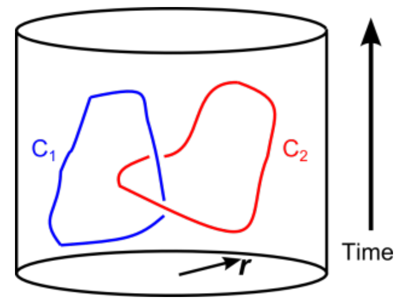


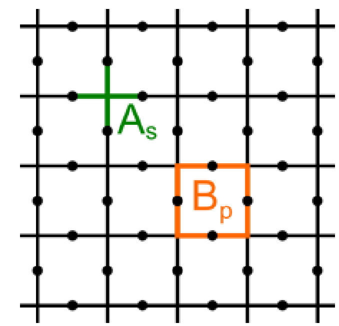
~~Exactly solvable~~ lattice model:



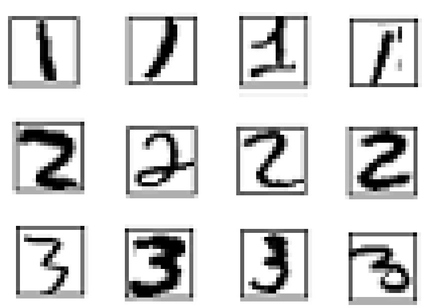
The ‘good’ versus the ‘not-so-good’

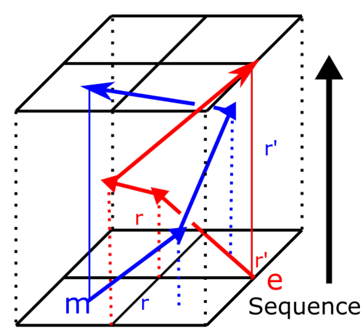
- The ‘good’: pristine data

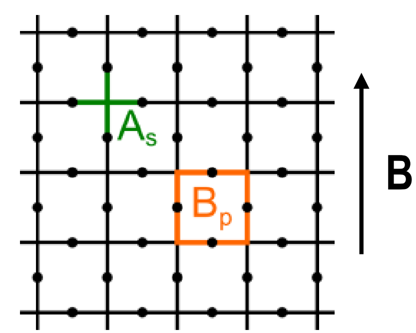




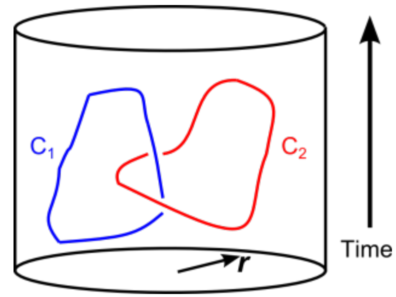
- The ‘not-so-good’: noisy data

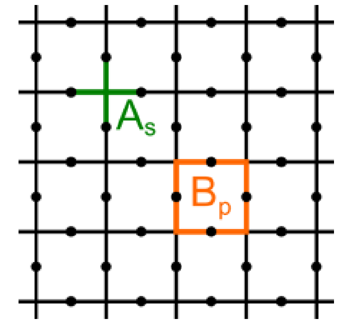




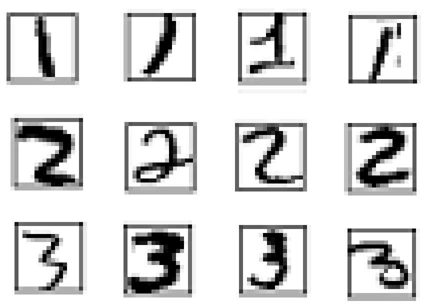


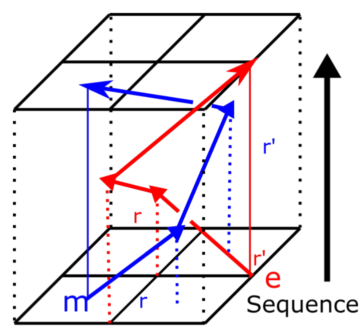
Option #1: suppress the noise

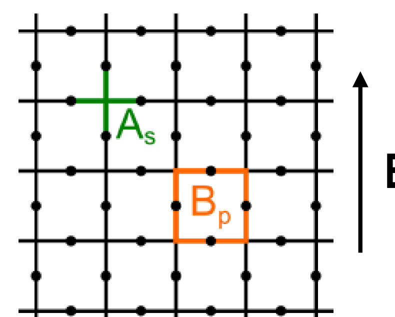




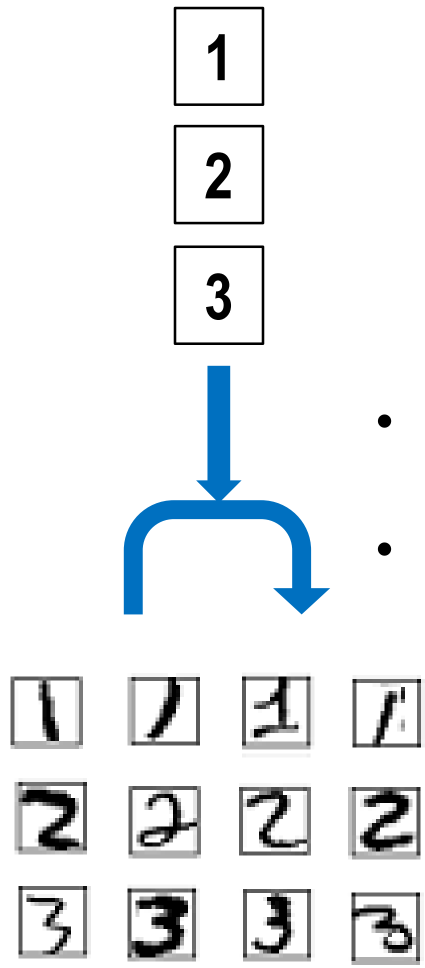
- Get rid of the noise and compare with existing knowledge
- However, sometimes expensive or unable

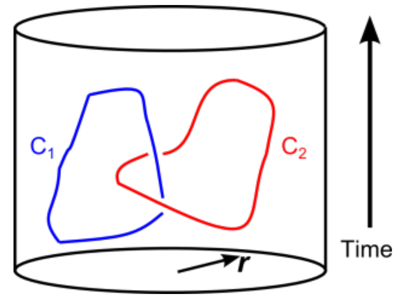


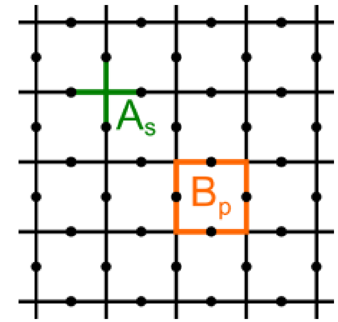




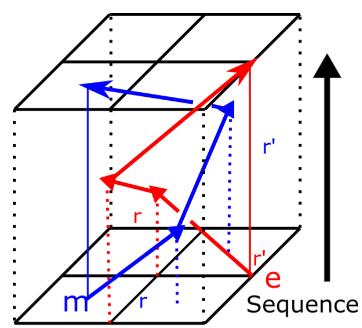
Option #2: learn from the noise

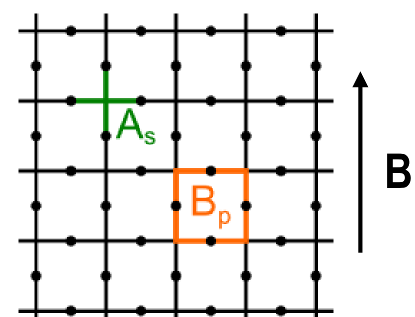






- Offer guidance – QLT
- Train with the noise to deal with the noise





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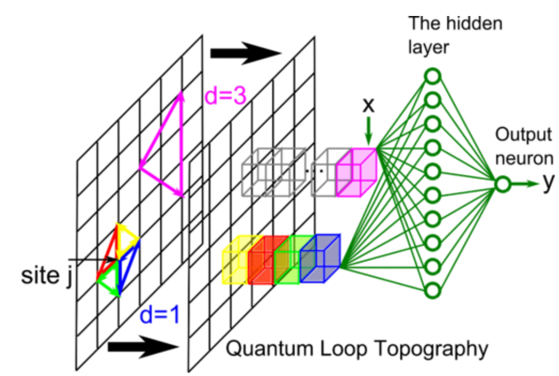
INTERPRETING THE PHYSICS

The physics underlying a phase

- First, make sure the trained machine learning architecture reflects the universality of the phase
  - e.g. phase diagram matches

- Then, ‘reverse engineer’ the architecture to formulate the function from input to output
  - Taylor expansion (sigmoid neurons)
  - Trace RELU firing (rectified linear neurons)



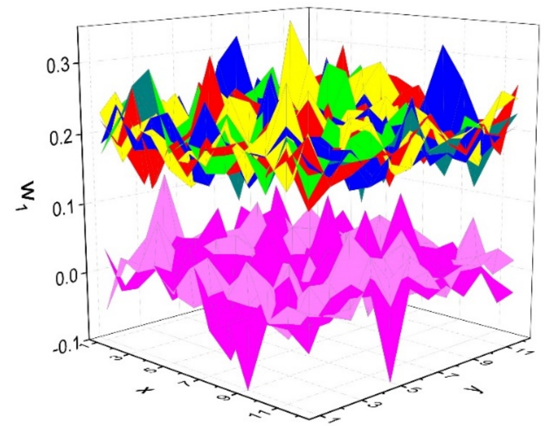
$f(x) = y$

Interpreting the QH insulator criteria

Firing condition of the output neuron:

Weights of the imaginary parts of the four smallest loops

Weights of the rest



$$-4.84 \times max\left[0.208 \sum_{dc=1} \mathrm{i}P_{jk}P_{kl}P_{lj} + 3.73,0\right] + 9.03 > 0$$

$$\frac{1}{N}\sum_{dc=1} 2\pi \mathrm{i}P_{jk}P_{kl}P_{lj} > 0.4$$

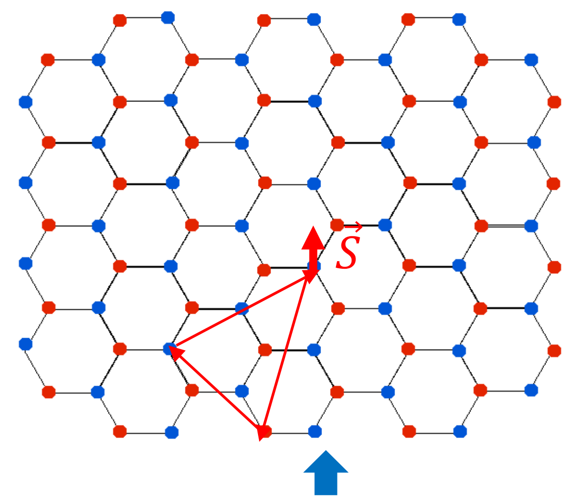
In comparison with: $\sigma_{xy} = \frac{e^2}{h} \cdot \frac{1}{N} \sum 4\pi i P_{jk} P_{kl} P_{lj} S_{\triangle jkl}$

S=1/2 for d_c=1

Example #3: quantum spin Hall insulator

$$H = t\sum_{\langle ij\rangle} c_i^\dagger c_j + i\lambda_{SO}\sum_{\langle\langle ij\rangle\rangle} \nu_{ij} c_i^\dagger s^z c_j + i\lambda_R \sum_{\langle ij\rangle} c_i^\dagger (\mathbf{s}\times\hat{\mathbf{d}}_{ij})_z c_j + \lambda_v \sum_i \xi_i c_i^\dagger c_i$$

C.L. Kane, E.J. Mele (2005)



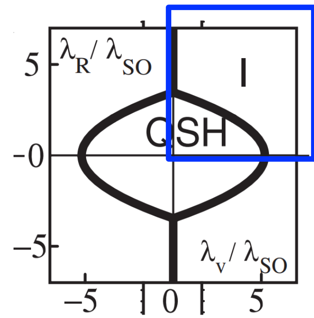
Include s_x , s_y and s_z

Intuition from spin Hall transport:

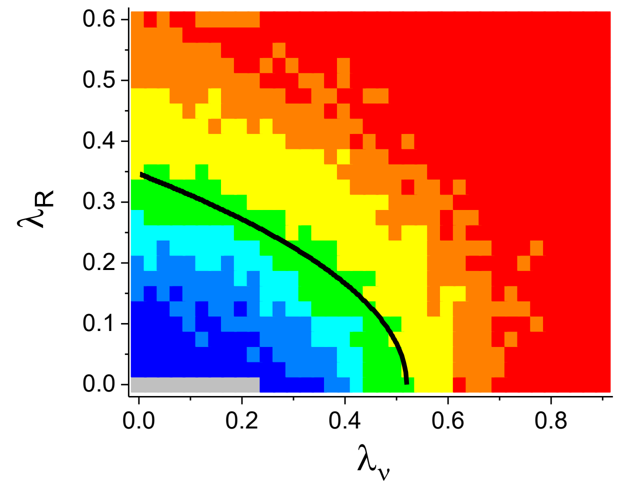
$tr(P[P,x\vec{s}][P,y])$

versus Hall transport: $tr(P[P,x][P,y])$

Phase diagram from machine learning



C.L. Kane, E.J. Mele (2005)



Phase diagram from neural outputs

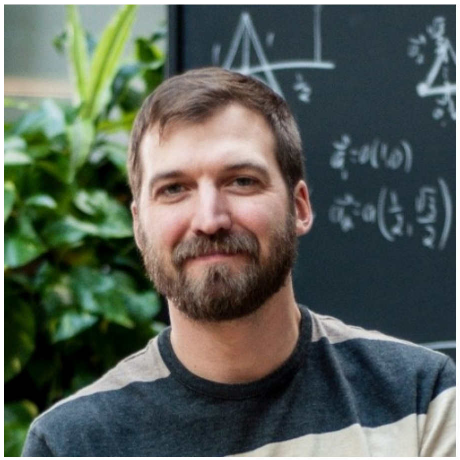
Map out the firing condition of the output neuron:

$$\sum_{d=x,y,z}\left(\sum Im[s_j^d P_{jk}P_{kl}P_{lj}S_{\Delta jkl}]\right)^2$$

From the 1st and 2nd smallest triangles

Calculated expectation value

Acknowledgement



Roger G. Melko

Eun-Ah Kim

Simon Trebst

Peter Broecker

Carsten Bauer

Michael Matty

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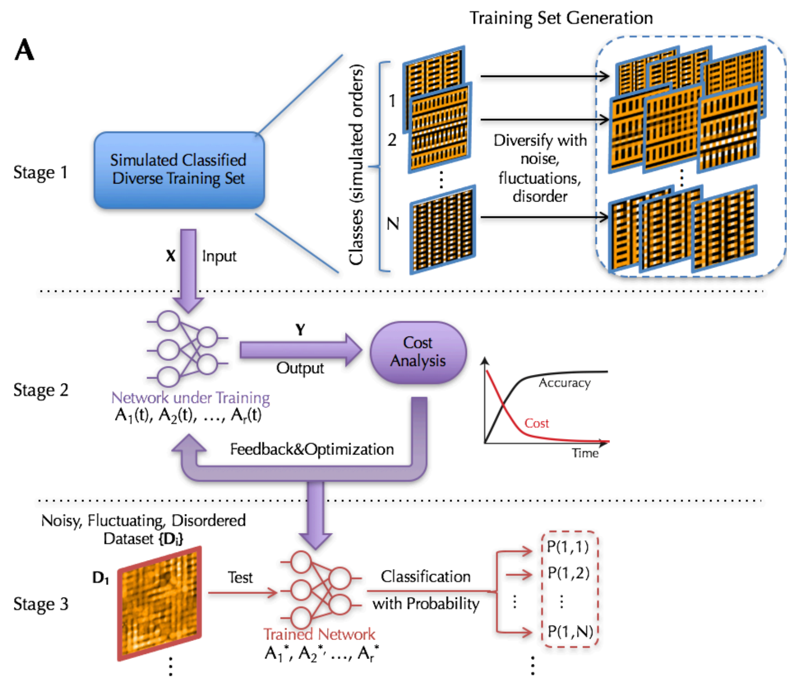
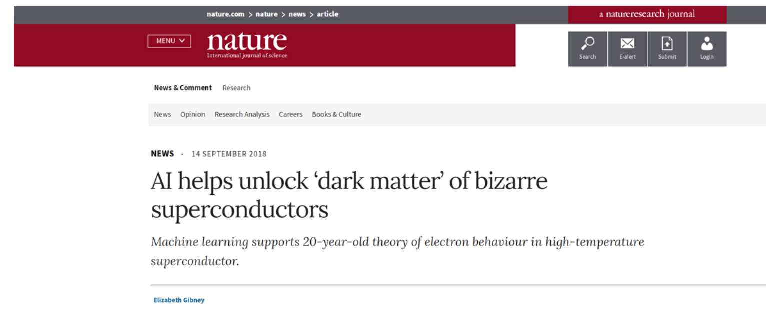
Paul Ginsparg

Interface between experiments and hypothetical theories

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NEWS · 14 SEPTEMBER 2018

AI helps unlock 'dark matter' of bizarre superconductors

Machine learning supports 20-year-old theory of electron behaviour in high-temperature superconductor.

Elizabeth Gibney

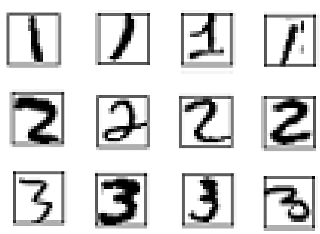
YZ, A. Mesaros, K. Fujita, S.D. Edkins, M.H. Hamidian, K. Ch'ng, H. Eisaki, S. Uchida, J.C. Séamus Davis, E. Khatami, E.-A. Kim (2018)

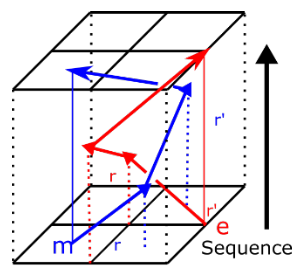
J.B. Goetz, YZ, M.J. Lawler (2019)

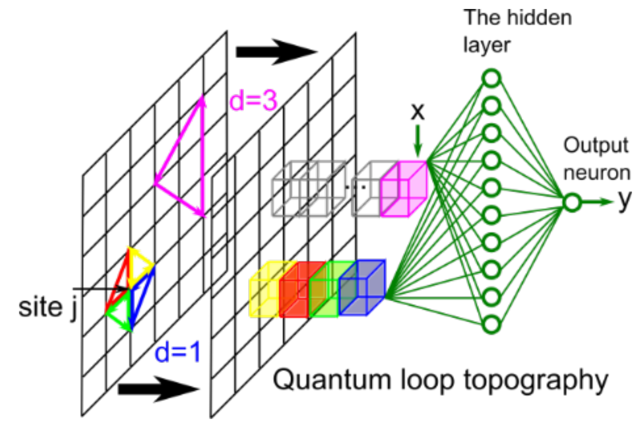
Summary

'Noisy' data

Informative 'operators'







Quantum systems ⟷ Quantum loop topography ⟷ Machine learning